

ABSTRACT

The present invention relates to a data storage medium encoded with the corresponding structure coordinates of molecules and molecular complexes which comprise the active site binding pockets of IMPDH. Such data storage material is capable of displaying such molecules and molecular complexes, or their structural homologues, as a graphical three-dimensional representation on a computer screen. This invention also relates to methods of using the structure coordinates to solve the structure of homologous proteins or protein complexes. In addition, this invention relates to methods of using the structure coordinates to screen and design compounds, including inhibitory compounds, that bind to IMPDH or homologues thereof. This invention also relates to molecules and molecular complexes which comprise the active site binding pockets of IMPDH or close structural homologues of the active site binding pockets. This invention also relates to compounds and pharmaceutical compositions which are inhibitors of IMPDH.